FILE 'HOME' ENTERED AT 16:29:10 ON 13 MAY 2005

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:29:19 ON 13 MAY 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 MAY 2005 HIGHEST RN 850400-93-0
DICTIONARY FILE UPDATES: 12 MAY 2005 HIGHEST RN 850400-93-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

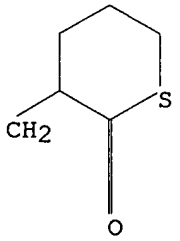
Please note that search-term pricing does apply when conducting SmartSELECT searches.

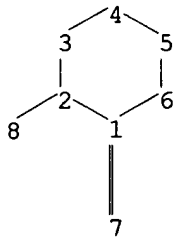
****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10791278.str





chain nodes :
7 8
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 2-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-7 2-3 3-4 4-5 5-6

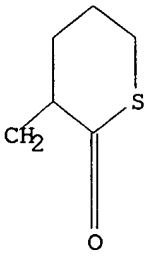
exact bonds :
2-8

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS

L1 STRUCTURE UPLOADED

=> s
ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end
SEARCH ENDED BY USER

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 16:29:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 162 TO ITERATE

100.0% PROCESSED 162 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2477 TO 4003
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 16:29:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3528 TO ITERATE

100.0% PROCESSED 3528 ITERATIONS 40 ANSWERS
SEARCH TIME: 00.00.01

L3 40 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 16:29:42 ON 13 MAY 2005

FILE COVERS 1907 - 13 May 2005 VOL 142 ISS 21
FILE LAST UPDATED: 12 May 2005 (20050512/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 25 L3

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 123.50 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

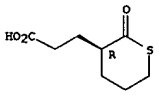
L4 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:154385 CAPLUS
DOCUMENT NUMBER: 142:348878
TITLE: Enantiospecificity of Glutamate Carboxypeptidase II Inhibition
AUTHOR(S): Tsukamoto, Takashi; Majer, Pavel; Vitharana, Dilruksh; Ni, Chiyou; Hin, Bunda; Lu, Xi-Chun M.; Thomas, Ajit G.; Wozniak, Krystyna M.; Calvin, David C.; Wu, Ying; Slusher, Barbara S.; Scarpetti, David; Bonneville, George W.
CORPORATE SOURCE: Guilford Pharmaceuticals Inc., Baltimore, MD, 21224, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(7), 2319-2324
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two representative glutamate carboxypeptidase II (GCP II) inhibitors, 2-(hydroxypentafluorophenylmethyl-phosphinoylmethyl)pentanedioic acid 2 and 2-(3-mercaptopropyl)pentanedioic acid 3, were synthesized in high optical purities (>97%ee). The two enantiomers of 2 were prepared from previously reported chiral intermediates, (R)- and (S)-2-(hydroxyphosphinoylmethyl)pentanedioic acid benzyl esters 8. The synthesis of (R)- and (S)-3 involves the hydrolysis of (R)- and (S)-3-(2-oxo-tetrahydro-thiopyran-3-yl)propionic acids, (R)- and (S)-11, the corresponding optically pure thiolactones delivered by chiral chromatog. separation of the racemic 11. GCP II inhibitory assay revealed that (S)-2 is 40-fold more potent than (R)-2. In contrast, both enantiomers of 3 inhibited GCP II with nearly equal potency. The efficacy observed in subsequent animal studies with these enantiomers correlated well with the inhibitory potency in a GCP II assay.

IT **848952-59-0P 848952-60-3P**
RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(glutamate carboxypeptidase II inhibitors preparation and enantiospecific activity)

RN 848952-59-0 CAPLUS
CN 2H-Thiopyran-3-propanoic acid, tetrahydro-2-oxo-, (3R)- (9CI) (CA INDEX NAME)

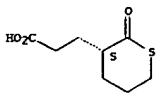
Absolute stereochemistry.



RN 848952-60-3 CAPLUS
CN 2H-Thiopyran-3-propanoic acid, tetrahydro-2-oxo-, (3S)- (9CI) (CA INDEX NAME)

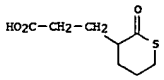
Absolute stereochemistry.

L4 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **757246-49-4P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(glutamate carboxypeptidase II inhibitors preparation and enantiospecific activity)

RN 757246-49-4 CAPLUS
CN 2H-Thiopyran-3-propanoic acid, tetrahydro-2-oxo- (9CI) (CA INDEX NAME)



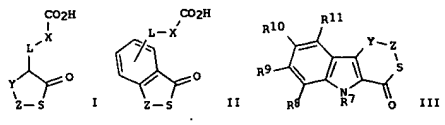
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Instant App

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:756706 CAPLUS
DOCUMENT NUMBER: 141:277490
TITLE: Preparation of thiolactone derivatives as inhibitors of NAALADase enzyme
INVENTOR(S): Tsukamoto, Takashi; Slusher, Barbara S.
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078742	A1	20040916	WO 2004-US6178	20040303
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005004203	A1	20050106	US 2004-791278	20040303
PRIORITY APPLN. INFO.:			US 2003-450648P P	20030303
OTHER SOURCE(S):	MARPAT 141:277490			

GI

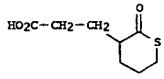


AB Title compds. represented by the formula I, II and III [wherein X = (un)substituted (cyclo)alkylene, (cyclo)alkenylene, alkynylene, (hetero)aryl; L = a bond, CR1R2, O, S, SO2, NR1; Y = O, S, CR3R4, NR3; Z = (CR5R6)n; n = 1-4; R1-R6 = independently H, (un)substituted alkyl, alkenyl; R7 = H, (un)substituted Ph, phenylethyl, benzyl; R8-R11 = independently H, carboxy, hydroxy, halo, nitro, cyano, alkyl, alkoxy; and pharmaceutically acceptable equivalent, an optical isomer or a mixture of isomers thereof] were prepared as NAALADase enzyme inhibitors. For example, cyclization of 2-[3-(tritylthio)mercaptopropyl]pentanedioic acid in acidic condition gave 3-(2-oxotetrahydrothiopyran-3-yl)propionic acid (IV) in 37% yield. 2-(3-Sulfanylpropyl)pentanedioic acid was tested for inhibition of NAALADase enzyme activity in treatment of retinal disorders, and IV was tested for protective effect of NAALADase inhibitors in exptl. rat glaucoma. Thus, this invention provided new compds., pharmaceutical compns. and diagnostic kits comprising such compds., and methods of using

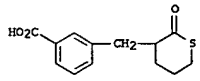
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
such compds. for inhibiting NAALADase enzyme activity, detecting diseases where NAALADase levels are altered, inhibiting angiogenesis, effecting a TGF-β activity or a neuronal activity, and treating a glutamate abnormality, a compulsive disorder, neuropathy, pain, a prostate disease, cancer, Huntington's disease, diabetes, a retinal disorder or glaucoma.

IT **757246-49-4P 757246-50-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiolactones as inhibitors of NAALADase enzyme)

RN 757246-49-4 CAPLUS
CN 2H-Thiopyran-3-propanoic acid, tetrahydro-2-oxo- (9CI) (CA INDEX NAME)



RN 757246-50-7 CAPLUS
CN Benzoic acid, 3-[(tetrahydro-2-oxo-2H-thiopyran-3-yl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

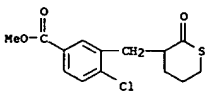
L4 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:555453 CAPLUS
DOCUMENT NUMBER: 137:124986
TITLE: Preparation of thiol-based NAALADase inhibitors and their uses thereof
INVENTOR(S): Tsukamoto, Takashi; Majer, Pavel; Stoermer, Doris; Slusher, Barbara S.
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 202 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057222	A2	20020725	WO 2002-US1205	20020117
WO 2002057222	A3	20021219		
WO 2002057222	C2	20040506		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2435273	AA	20020725	CA 2002-2435273	20020117
US 2003105088	A1	20030605	US 2002-46917	20020117
US 6586623	B2	20030701		
EP 1353903	A2	20031022	EP 2002-713419	20020117
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004524294	T2	20040812	JP 2002-557903	20020117
US 2003216468	A1	20031120	US 2003-431462	20030508
US 6812364	B2	20041102		
US 2005085503	A1	20050421	US 2004-959199	20041007

PRIORITY APPLN. INFO.: US 2001-261754P P 20010117
US 2001-342772P P 20011228
US 2002-46917 A3 20020117
WO 2002-US1205 W 20020117
US 2003-431462 A3 20030508

OTHER SOURCE(S): MARPAT 137:124986
AB This invention relates to new compds., pharmaceutical compns. and diagnostic kits comprising such compds., and methods of using such compds. for inhibiting NAALADase enzyme activity, detecting diseases where NAALADase levels are altered, effecting neuronal activity, effecting TGF-b activity, inhibiting angiogenesis, and treating glutamate abnormalities, diabetic neuropathy, pain, compulsive disorders, prostate diseases, cancers and glaucoma. Thus, rats treated with NAALADase inhibitor 3-carboxy-5-(1,1-dimethylethyl)-alpha-(3-mercaptopropyl)benzenepropanoic acid of this invention at various dose levels (10, 1, 0.1 mg/kg) for 15 days after sciatic nerve ligation showed normalized difference in scores between the operated and unoperated paws compared to continued hyperalgesic for rats treated with vehicle under the same conditions.
IT **377731-27-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

L4 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(in prepn. and uses of thiol-based NAALADase inhibitors)
RN 377731-27-6 CAPLUS
CN Benzoic acid, 4-chloro-3-[(tetrahydro-2-oxo-2H-thiopyran-3-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

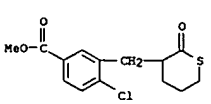


L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:886142 CAPLUS
DOCUMENT NUMBER: 136:15255
TITLE: NAALADase inhibitors for treating retinal disorders and glaucoma
INVENTOR(S): Slusher, Barbara S.; Wozniak, Krystyna
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 196 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092274	A2	20011206	WO 2001-US17288	20010530
WO 2001092274	A3	20020530		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2410889	AA	20011206	CA 2001-2410889	20010530
US 2003036534	A1	20030220	US 2001-866961	20010530
EP 1292601	A2	20030319	EP 2001-944182	20010530
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003535098	T2	20031125	JP 2002-500887	20010530

PRIORITY APPLN. INFO.: US 2000-207320P P 20000530
WO 2001-US17288 W 20010530

OTHER SOURCE(S): MARPAT 136:15255
AB The invention discloses pharmaceutical compns. and methods for treating a retinal disorder or glaucoma using NAALADase inhibitors.
IT **377731-27-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction; NAALADase inhibitors for treating retinal disorders and glaucoma)
RN 377731-27-6 CAPLUS
CN Benzoic acid, 4-chloro-3-[(tetrahydro-2-oxo-2H-thiopyran-3-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

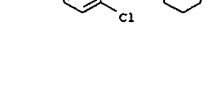


L4 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:885736 CAPLUS
DOCUMENT NUMBER: 136:15243
TITLE: NAALADase inhibitors for treating amyotrophic lateral sclerosis
INVENTOR(S): Slusher, Barbara S.; Wozniak, Krystyna
PATENT ASSIGNEE(S): Guilford Pharmaceuticals Inc., USA
SOURCE: PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001091738	A2	20011206	WO 2001-US17325	20010530
WO 2001091738	A3	20020906		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002013295	A1	20020131	US 2001-866729	20010530

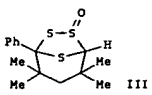
PRIORITY APPLN. INFO.: US 2000-207319P P 20000530

OTHER SOURCE(S): MARPAT 136:15243
AB The invention discloses pharmaceutical compns. and methods for treating amyotrophic lateral sclerosis using NAALADase inhibitors.
IT **377731-27-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction; NAALADase inhibitors for treating amyotrophic lateral sclerosis)
RN 377731-27-6 CAPLUS
CN Benzoic acid, 4-chloro-3-[(tetrahydro-2-oxo-2H-thiopyran-3-yl)methyl]-, methyl ester (9CI) (CA INDEX NAME)

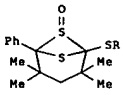


L4 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

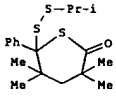
ACCESSION NUMBER: 1999:548678 CAPLUS
DOCUMENT NUMBER: 131:299188
TITLE: Rearrangement of the carbanion generated from a tied-back 1,2,4-trithiolane oxide (6,7,8-trithiabicyclo[3.2.1]octane 6-oxide)
AUTHOR(S): Ishii, Akihiko; Nakaniwa, Tetsuya; Umezawa, Kazuyo; Nakayama, Juzo
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Saitama University, Saitama, 338-8570, Japan
SOURCE: Tetrahedron (1999), 55(34), 10341-10350
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



III



XII



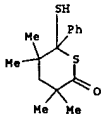
XIV

AB Treatment of 2,2,4,4-tetramethyl-6,7,8-trithiabicyclo[3.2.1]octane 6-exo-oxide (III) with LDA, followed by treatment with D2O, RI (R = Me, Et), and 2-PrBr, yielded the bridgehead-deuterated starting compound, bicyclic 1,3-dithietane oxides (XII), and (2-propyldithio)thiolactone (XIV), resp. The initially-formed bridgehead lithium salt opens the bicyclic skeleton to give the lithium δ-thioxoperoxydithiocarboxylate, which finally isomerizes to the lithium (3-oxo-2-thianyl)disulfide via the peroxydithiocarboxylate-α-oxodisulfide rearrangement.

IT **247090-31-9P**
RL: FRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; rearrangement mechanism of the carbanion generated from a tied-back 1,2,4-trithiolane oxide (6,7,8-trithiabicyclo[3.2.1]octane 6-oxide))

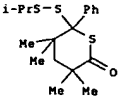
RN 247090-31-9 CAPLUS
CN 2H-Thiopyran-2-one, tetrahydro-3,3,5,5-tetramethyl-6-[(1-methylethyl)dithio]-6-phenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

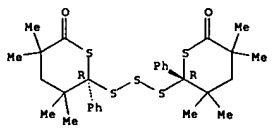
L4 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **247090-32-0P 247090-33-1P 247090-34-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(rearrangement mechanism of the carbanion generated from a tied-back 1,2,4-trithiolane oxide (6,7,8-trithiabicyclo[3.2.1]octane 6-oxide))

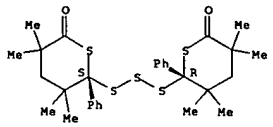
RN 247090-32-0 CAPLUS
CN 2H-Thiopyran-2-one, 6,6'-trithiobis[tetrahydro-3,3,5,5-tetramethyl-6-phenyl-, (6R,6'R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 247090-33-1 CAPLUS
CN 2H-Thiopyran-2-one, 6,6'-trithiobis[tetrahydro-3,3,5,5-tetramethyl-6-phenyl-, (6R,6'S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 247090-34-2 CAPLUS
CN 2H-Thiopyran-2-one, tetrahydro-6-mercapto-3,3,5,5-tetramethyl-6-phenyl- (9CI) (CA INDEX NAME)

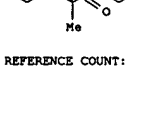
L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:435173 CAPLUS
DOCUMENT NUMBER: 129:122309
TITLE: In search for thioketene S-oxide. A vinyl sulfoxide to sulfine rearrangement
AUTHOR(S): Pelloux-Leon, Nadia; Minassian, Frederic; Levillain, Jocelyne; Ripoll, Jean-Louis; Vallee, Yannick
CORPORATE SOURCE: L.E.D.S.S., CNRS et Universite Joseph Fourier, Grenoble, 38041, Fr.
SOURCE: Tetrahedron Letters (1998), 39(27), 4813-4816
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two approaches to thioketene S-oxide have been tested. This reactive heterocumulene was tentatively characterized by low temperature IR spectroscopy.
In the course of this study, an unexpected vinyl sulfoxide to sulfine rearrangement was observed

IT **210405-52-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(attempted methylenation with Tebbe reagent; formation of thioketene S-oxide by flash vacuum thermolysis of retro Diels-Alder precursors and observation of a vinyl sulfoxide to sulfine rearrangement)

RN 210405-52-0 CAPLUS
CN 10,9-(Epithiomethano)anthracen-12-one, 9,10-dihydro-9,10-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

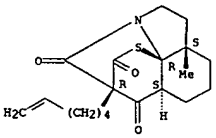
ACCESSION NUMBER: 1995:807384 CAPLUS
DOCUMENT NUMBER: 124:29686
TITLE: On the intramolecular 1,4-dipolar cycloaddition reaction of thiazinium betaines for the construction of aza-, diaza-, and polyaza-heterocyclic ring systems
AUTHOR(S): Padwa, Albert; Coats, Steven J.; Harring, Scott R.; Hadjiarapoglou, Lazaros; Semones, Mark A.
CORPORATE SOURCE: Dep. Chemistry, Emory Univ., Atlanta, GA, 30322, USA
SOURCE: Synthesis (1995), (8), 973-84
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:29686

AB A series of bicyclic anhydro-4-hydroxy-2-oxo-1,3-thiazinium hydroxides containing tethered π-systems were easily prepared from the reaction of thiolactams with 1,3-bielectrophiles. These cross-conjugated heteroarom. betaines underwent regio- and stereospecific 1,4-dipolar cycloaddn. in good yield to produce cycloadducts containing a C(:O)S bridge which was induced to lose COS on further heating. Two of the cycloadducts were characterized by single crystal x-ray detns. Control of ring size in the final product of the cycloaddn. was achieved by variation of the dipolarophilic chain length. Entry to the [6,6,5]- and [6,6,6]-pyridone ring systems was possible with phenylalkynyl-substituted thioamides. Intramol. 1,4-dipolar cycloaddn. of a thiazinium betaine dipole also occurred across an indolyl π-bond. With only one substituent group in the 9-position of the bicyclic betaine, the reaction takes an entirely different course unless a highly activated π-bond is incorporated into the tether. The preferred reaction with modestly activated π-systems corresponds to loss of the activated H+ to produce an S,N-ketene acetal. When a ketene S,S-acetal group was incorporated onto the side chain, the 1,4-dipolar cycloaddn. reaction was facilitated relative to H+ loss.

IT 171616-38-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intramol. 1,4-dipolar cycloaddn. of thiazinium betaines for preparation of
aza-, diaza-, and polyaza-heterocyclic ring systems)

RN 171616-38-9 CAPLUS
CN 3,11-Methano-2H,6H-[1,3]thiazino[2,3-i]indole-2,4,12(3H)-trione, hexahydro-7a-methyl-3-(5-hexenyl)-, (3R,7aS,11S,11aR)-rel- (9CI) (CA INDEX NAME)

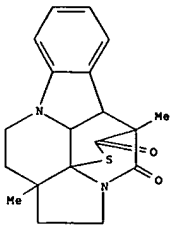
Relative stereochemistry.



IT 171616-52-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(intramol. 1,4-dipolar cycloaddn. of thiazinium betaines for preparation of

L4 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
aza-, diaza-, and polyaza-heterocyclic ring systems)

RN 171616-52-7 CAPLUS
CN 2H-1,11-Methanobenzo[b]pyrrolo[3,2-g]thiopyrano[2,3,4-hi]indolizine-12,14(11H)-dione, 3,3a,4,5,10b,13b-hexahydro-3a,11-dimethyl- (9CI) (CA INDEX NAME)



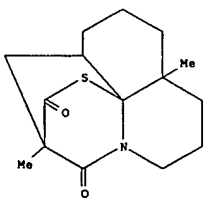
L4 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:761231 CAPLUS
DOCUMENT NUMBER: 123:339957
TITLE: 8H-anhydro-4-hydroxy-2-oxo-1,3-thiazinium hydroxides as mesoionic 1,4-dipoles
AUTHOR(S): Padwa, Albert; Coats, Steven J.; Hadjiarapogiou, Lazaros
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Heterocycles (1995), 41(8), 1631-52
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The previously unknown 8H-anhydro-4-hydroxy-2-oxo-1,3-thiazinium hydroxides were prepared, and their 1,4-dipolar cycloaddn. behavior was examined. In most cases, elimination of the proton in the 8-position of the mesoionic ring was observed to occur unless extremely reactive dipolarophiles were used. The S,N-ketene acetals were converted to the corresponding α-diazo ketones for further study.

IT 150989-36-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(anhydrohydroxyoxothiazinium hydroxides as mesoionic dipoles)

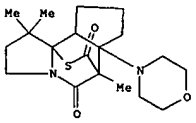
RN 150989-36-9 CAPLUS
CN 3,12-Methano-2H-[1,3]thiazino[2,3-j]quinoline-2,4(3H)-dione, octahydro-3,8a-dimethyl- (9CI) (CA INDEX NAME)



IT 153616-83-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(anhydrohydroxyoxothiazinium hydroxides as mesoionic dipoles)

RN 153616-83-2 CAPLUS
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-1,1,6-trimethyl-6a-(4-morpholinyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

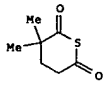


L4 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:658527 CAPLUS
DOCUMENT NUMBER: 123:227968
TITLE: Synthesis of small-medium ring thioanhydrides
AUTHOR(S): Kates, Michael J.; Schauble, J. Herman
CORPORATE SOURCE: Department of Chemistry, Villanova University, Villanova, PA, 19085, USA
SOURCE: Journal of Heterocyclic Chemistry (1995), 32(3), 971-8
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:227968

AB Reaction of five-membered ring anhydrides with sodium sulfide has previously been employed for synthesis of the corresponding thioanhydrides in low yields. Reexamn. of the stoichiometry reveals reaction of cyclic anhydride with sodium sulfide (2:1 resp.), affords the thioanhydride accompanied by the corresponding dicarboxylate in a 1:1 molar ratio. The mechanistic pathway for this reaction has also been elucidated. Optimization of reaction conditions has resulted in the synthesis of a variety of four to seven-membered ring thioanhydrides in yields approaching theor. The reaction of disodium sulfide with 1,1-cyclobutanedicarboxylic acid gave 2-thiaspiro[3.3]heptane-1,3-dione (74% yield). The reaction of 1,2-benzenedicarboxylic acid gave benzo[c]thiophene-1,3-dione.

IT **168280-83-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of small or medium-sized sulfur-containing heterocyclic compds.)

RN 168280-83-9 CAPLUS
CN 2H-Thiopyran-2,6(3H)-dione, dihydro-3,3-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:636851 CAPLUS
DOCUMENT NUMBER: 123:339780
TITLE: Details associated with the bimolecular 1,4-dipolar cycloaddition reaction of cross-conjugated heteroaromatic betaines
AUTHOR(S): Padwa, Albert; Coats, Steven J.; Semones, Mark A.
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA
SOURCE: Tetrahedron (1995), 51(24), 6651-68
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Pergamon
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:339780
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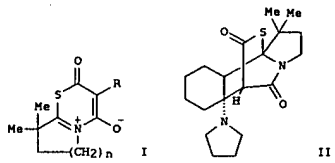


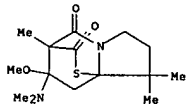
I II

AB A series of 3,3-disubstituted bicyclic anhydro-4-hydroxy-2-oxo-1,3-thiazinium hydroxides are easily prepared from the reaction of 3H-thiolactams with 1,3-bielectrophiles. These cross-conjugated heteroarom. betaines, e.g. I (R = Me, Ph; n = 1, 2), undergo regio- and diastereospecific 1,4-dipolar cycloaddn. with electron-rich and electron-deficient π-bonds to produce 1,4-cycloadducts containing a carbonyl sulfide bridge. A representative betaine dipole (I, R = Ph, n = 2) and 1,4-cycloadduct (II) were characterized by single crystal X-ray detns. In certain cases, the initially formed cycloadduct can be induced to lose COS on further heating. The frontier orbital coeffs. of the thiazinium betaine were determined by semiempirical MOPAC calcns. with the PM3 Hamiltonian. The HOMO of the 1,4-dipole is dominant for reactions with electron-deficient dipolarophiles such as N-phenylmaleimide, while the LUMO becomes important for cycloaddn. to more electron-rich species such as ynamines or vinyl ethers.

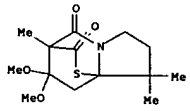
IT **153616-74-1P 153616-76-3P 170449-62-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bimol. 1,4-dipolar cycloaddn. reaction of cross-conjugated heteroarom. betaines)

RN 153616-74-1 CAPLUS
CN 6H-3,8a-Ethano-2H-pyrrolo[2,1-b][1,3]thiazine-2,4(3H)-dione, 10-(dimethylamino)dihydro-10-methoxy-3,8,8-trimethyl- (9CI) (CA INDEX NAME)

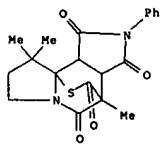
L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 153616-76-3 CAPLUS
CN 6H-3,8a-Ethano-2H-pyrrolo[2,1-b][1,3]thiazine-2,4(3H)-dione, dihydro-10,10-dimethoxy-3,8,8-trimethyl- (9CI) (CA INDEX NAME)



RN 170449-62-4 CAPLUS
CN 7H-9a,4-(Epithiomethano)-1H-pyrrolo[3,4-g]indolizine-1,3,5,11(2H,4H)-tetrone, tetrahydro-4,9,9-trimethyl-2-phenyl- (9CI) (CA INDEX NAME)

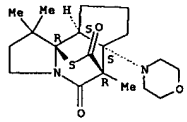


IT **166734-35-6P 170449-63-5P 170449-67-9P**
170555-54-1P 170555-55-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(bimol. 1,4-dipolar cycloaddn. reaction of cross-conjugated heteroarom. betaines)

RN 166734-35-6 CAPLUS
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-1,1,6-trimethyl-6a-(4-morpholinyl)-, (6α,6aβ,9aβ,9bα)- (9CI) (CA INDEX NAME)

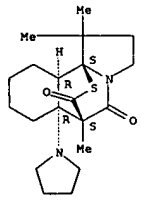
Relative stereochemistry.

L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

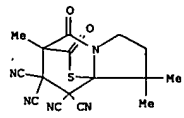


RN 170449-63-5 CAPLUS
CN 1H-10b,6-(Epithiomethano)pyrrolo[2,1-a]isoquinoline-5,12(6H)-dione, octahydro-1,1,6-trimethyl-6a-(1-pyrrolidinyl)-, (6α,6aβ,10aβ,10bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



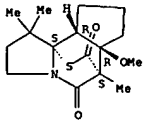
RN 170449-67-9 CAPLUS
CN 6H-3,8a-Ethano-2H-pyrrolo[2,1-b][1,3]thiazine-9,9,10,10-tetracarbonitrile, tetrahydro-3,8,8-trimethyl-2,4-dioxo- (9CI) (CA INDEX NAME)



RN 170555-54-1 CAPLUS
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-6a-methoxy-1,1,6-trimethyl-, (6α,6aβ,9aβ,9b.alph a.)- (9CI) (CA INDEX NAME)

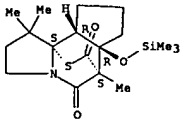
Relative stereochemistry.

L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



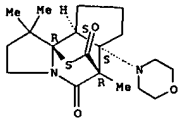
RN 170555-55-2 CAPLUS
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-1,1,6-trimethyl-6a-[(trimethylsilyl)oxy]-, (6α,6aβ,9aβ,9bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

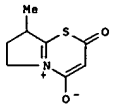


L4 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-1,1,6-trimethyl-6a-(4-morpholinyl)-, (6α,6aβ,9aβ,9bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

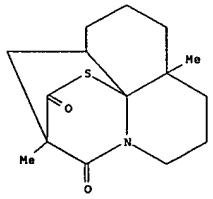


L4 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:326747 CAPLUS
DOCUMENT NUMBER: 123:143771
TITLE: 8H-Anhydro-4-hydroxy-2-oxo-1,3-thiazinium hydroxides as mesoionic 1,4-dipoles
AUTHOR(S): Padwa, Albert; Coats, Steven J.; Hadjiarapoglou, Lazaros
CORPORATE SOURCE: Department of Chemistry, Emory Univ., Atlanta, GA, 30322, USA
SOURCE: Heterocycles (1994), 39(1), 219-41
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The title compds., e.g., I, were prepared, and their 1,4-dipolar cycloaddn. behavior was examined In most cases, elimination of a ring proton occurred unless extremely reactive dipolarophiles were used. The S,N-ketene acetals were converted to the corresponding α-diazo ketones for further study.
IT **150989-36-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cycloaddn. reaction of hydroxyoxothiazinium inner salts)
RN 150989-36-9 CAPLUS
CN 3,12-Methano-2H-[1,3]thiazino[2,3-j]quinoline-2,4(3H)-dione, octahydro-3,8a-dimethyl- (9CI) (CA INDEX NAME)

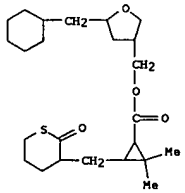


IT **166734-35-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 166734-35-6 CAPLUS

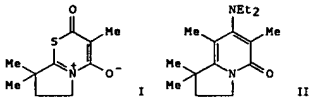
L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:275031 CAPLUS
DOCUMENT NUMBER: 122:74619
TITLE: Pesticide for preventing and eliminating pests with high pesticide resistance
INVENTOR(S): Liu, Runxi
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 18 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1081063	A	19940126	CN 1992-105309	19920706
PRIORITY APPLN. INFO.:			CN 1992-105309	19920706

AB The pesticide is prepared from oxime group-containing bactericides 3-10 weight%, heterocyclic pyrethrin 10-20, F-containing or heterocyclic pyrethrin 3-5, diesel oil 30-36, first emulsifier 4-5, second emulsifier 4-5, solvent 9-36., and enhanced P SV1 10.
IT **160219-71-6**, Saienjuzhi
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(pesticide for preventing and eliminating pests with high pesticide resistance)
RN 160219-71-6 CAPLUS
CN Cyclopropanecarboxylic acid, 2,2-dimethyl-3-[(tetrahydro-2-oxo-2H-thiopyran-3-yl)methyl]-, [5-(cyclohexylmethyl)tetrahydro-3-furanyl]methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:217200 CAPLUS
DOCUMENT NUMBER: 120:217200
TITLE: Bimolecular [4+2]-cycloaddition reactions of cross conjugated betaines with electron rich π-systems
AUTHOR(S): Padwa, Albert; Coats, Steven J.; Semones, Mark A.
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA
SOURCE: Tetrahedron Letters (1993), 34(34), 5405-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:217200
GI

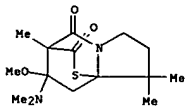


I II

AB Bicyclic anhydro-2-oxo-4-hydroxy-1,3-thiazinium hydroxides undergo 1,4-dipolar cycloaddns. with various electron rich π-systems to give 4+2-cycloadducts which on further heating, extrude carbonyl sulfide producing substituted α-pyridones. The cycloaddn. of 1-(diethylamino)-1-propyne with the (oxo)hydroxythiazinium hydroxide I gave the bicyclic α-pyridone II in 100% yield.

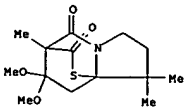
IT **153616-74-1P 153616-76-3P 153616-79-6P 153616-80-9P 153616-82-1P 153616-83-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, α-pyridone by 1,4-dipolar cycloaddn. of (oxo)hydroxythiazinium hydroxide with electron-rich π system)

RN 153616-74-1 CAPLUS
CN 6H-3,8a-Ethano-2H-pyrrolo[2,1-b][1,3]thiazine-2,4(3H)-dione, 10-(dimethylamino)dihydro-10-methoxy-3,8,8-trimethyl- (9CI) (CA INDEX NAME)

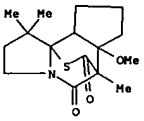


RN 153616-76-3 CAPLUS
CN 6H-3,8a-Ethano-2H-pyrrolo[2,1-b][1,3]thiazine-2,4(3H)-dione, dihydro-10,10-dimethoxy-3,8,8-trimethyl- (9CI) (CA INDEX NAME)

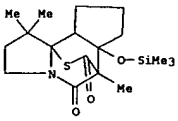
L4 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



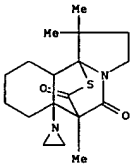
RN 153616-79-6 CAPLUS
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-6a-methoxy-1,1,6-trimethyl- (9CI) (CA INDEX NAME)



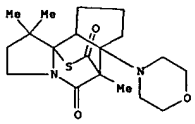
RN 153616-80-9 CAPLUS
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-1,1,6-trimethyl-6a-[(trimethylsilyl)oxy]- (9CI) (CA INDEX NAME)



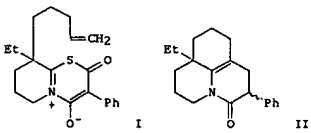
RN 153616-82-1 CAPLUS
CN 1H-10b,6-(Epithiomethano)pyrrolo[2,1-a]isoquinoline-5,12(6H)-dione, 6a-(1-aziridinyl)octahydro-1,1,6-trimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 153616-83-2 CAPLUS
CN 5H-9b,6-(Epithiomethano)-1H-cyclopent[g]indolizine-5,11-dione, octahydro-1,1,6-trimethyl-6a-(4-morpholinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1993:650217 CAPLUS
DOCUMENT NUMBER: 119:250217
TITLE: Intramolecular 1,4-dipolar cycloaddition of cross-conjugated heterocyclic betaines. A new route to hexahydrojulolidines and related peri-fused ring systems
AUTHOR(S): Potts, Kevin T.; Rochanapruk, Thevarak; Coats, Steven J.; Hadjiarapoglou, Lazaros; Padwa, Albert
CORPORATE SOURCE: Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12181, USA
SOURCE: Journal of Organic Chemistry (1993), 58(19), 5040-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:250217
GI



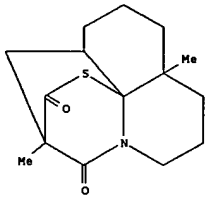
I II

AB Bicyclic anhydro-4-hydroxy-2-oxo-1,3-thiazinium hydroxides which were disubstituted in the 9-position with alkyl groups and alkenyl side-chains of suitable length, e.g. I, were obtained from the appropriately substituted thiolactams and 1,3-bielectrophiles. Upon heating, these betaines gave intramol. cycloadducts which underwent thermal loss of carbonyl sulfide, followed by a 1,5-hydrogen shift, to form hexahydrojulolidines, e.g. II, and related ring systems in generally good yields. Locating the dipolarophilic side-chain in the 3-position of the 1,4-dipole allowed the construction of linear, tricyclic ring-fused systems.

IT **150989-36-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal elimination of)

RN 150989-36-9 CAPLUS
CN 3,12-Methano-2H-[1,3]thiazino[2,3-j]quinoline-2,4(3H)-dione, octahydro-3,8a-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L4 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:128799 CAPLUS
DOCUMENT NUMBER: 116:128799
TITLE: Reaction of thioketones with carbonyl oxides and 3,3-dimethyl-1,2-dioxirane. [3 + 2] Cycloaddition vs. oxygen atom transfer
AUTHOR(S): Tabuchi, Toshihiko; Nojima, Masatomo; Kusabayashi, Shigekazu
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Osaka, 565, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1991), (12), 3043-6
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:128799
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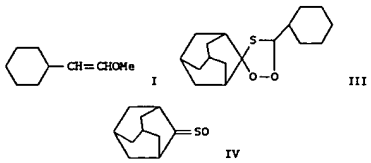


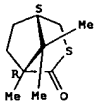
AB The ozonolysis of vinyl ethers, e.g., I, in the presence of adamantane-2-thione (II) and bicyclo[3.3.1]nonane-9-thione gave in each case the corresponding thioozonides, e.g., III in moderate yield, while ozonolysis of a mixture of vinyl ethers and thiobenzophenone derivs, such as, (4-MeC6H4)2CS, gave the corresponding thione S-oxides in isolated yields of 10-40%, together with the benzophenones. 3,3-Dimethyl-1,2-dioxirane, generated in situ from the reaction of acetone and oxone (2KHSO5-KHSO4-K2SO4), transferred an oxygen atom to compds. thiones, e.g., II, providing the thione S-oxides, such as, IV, in 29-97% yield.

IT 139483-06-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 139483-06-0 CAPLUS

CN 3-Thiabicyclo[3.2.1]octan-2-one, 1,8,8-trimethyl-, (1R)- (9CI) (CA INDEX NAME)

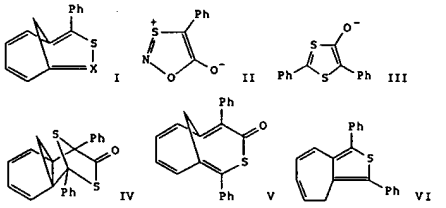
Absolute stereochemistry.



L4 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L4 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:631349 CAPLUS
DOCUMENT NUMBER: 113:231349
TITLE: Heterocycles by cycloaddition. Part 9. Bridged heteroannulenes by cycloaddition-extrusion-ring-expansion reactions of mesoionic compounds with benzocyclopropene. A methanothiazonine, a methanothionine, and a methanothiecinone
AUTHOR(S): Kato, Hiroshi; Toda, Shigeo; Arikawa, Yukihiko; Masuzawa, Mayumi; Hashimoto, Masafumi; Ikoma, Keiko; Wang, Shu Zhong; Miyasaka, Akemi
CORPORATE SOURCE: Fac. Sci., Shinshu Univ., Matsumoto, 390, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1990), (7), 2035-40
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:231349
GI



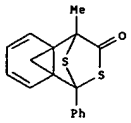
AB A methanothiazonine (I; X = N) was formed by cycloaddn.-extrusion-ring expansion of benzocyclopropene with a mesoionic oxathiazoliumolate (II). The reaction with a dithioliumolate (III) gave the cycloadduct (IV), from which a methanothionine (I; X = CPh) and a methanothiecinone (V) were prepared Attempts at similar reactions with several other mesoionic systems either failed to give the cycloadducts, or the cycloadducts did not form the desired extrusion products. The methanothionine (I; X = CPh) isomerized thermally to a cycloheptathiophene (VI). The degree of electron delocalization of these bridged annulenes is discussed.

IT 130520-11-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 130520-11-5 CAPLUS

CN 1,4-Epithio-4a,8a-methano-1H-2-benzothiopyran-3(4H)-one, 4-methyl-1-phenyl-, (1α,4α,4aα,8aα)- (9CI) (CA INDEX NAME)

L4 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

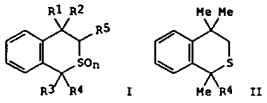


L4 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:156277 CAPLUS
DOCUMENT NUMBER: 106:156277
TITLE: Benzothiopyran derivatives
INVENTOR(S): Hori, Mikio; Kataoka, Sada; Kurono, Masatsune; Shimizu, Hiroshi; Iwata, Noriyuki; Imai, Eiji; Koide, Tokuo; Kawamura, Norihiro
PATENT ASSIGNEE(S): Sanwa Kagaku Kenkyusho Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61227580	A2	19861009	JP 1985-68419	19850402
JP 05041151	B4	19930622		
PRIORITY APPLN. INFO.:			JP 1985-68419	19850402

OTHER SOURCE(S): CASREACT 106:156277
GI

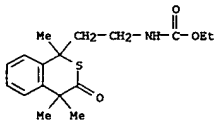


AB Benzothiopyran derivs. (I; R1, R2, R3 = alkyl; R4 = cyano, CO2H, hydroxyalkyl, etc.; R5 = H, AcO; R4R5 = CH2CH2NR6 where R6 = alkyl, alkoxycarbonyl; n = 0, 1), effective analgesics (no data), are prepared Thus, hydrolysis of cyano compound II (R4 = cyano) gave 83.7% carboxylic acid II (R4 = CO2H), which was reduced with LiAlH4 to give 94.2% alc. II (R4 = CH2OH) (III). Chlorination of III followed by cyanation gave 64.1% cyano derivative II (R4 = CH2CN), which was reduced with LiAlH4 to give 86.9% ethylamine derivative II (R4 = CH2CH2NH2) (IV). Substitution of IV with ClCO2Et gave 93.7% II (R4 = CH2CH2NHCO2Et), which was oxidized with m-ClC6H4CO2OH to give 91.7% S-oxide I (R1-3 = Me, R4 = CH2CH2NHCO2Et, R5 = H, n = 1).

IT 107026-55-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

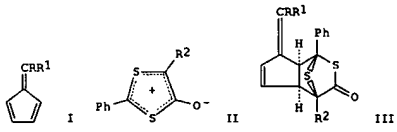
RN 107026-55-1 CAPLUS
CN Carbamic acid, [2-(3,4-dihydro-1,4,4-trimethyl-3-oxo-1H-2-benzothiopyran-1-yl)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L4 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:5804 CAPLUS
DOCUMENT NUMBER: 104:5804
TITLE: Heterocycles by cycloaddition. Part 7. Cycloaddition reactions of mesoionic dithiolones with fulvenes
AUTHOR(S): Kato, Hiroshi; Aoki, Nobuo; Kawamura, Yasuhiko; Yoshino, Kazue
CORPORATE SOURCE: Dep. Chem., Shinshu Univ., Matsumoto, 390, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (6), 1245-7
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:5804
GI

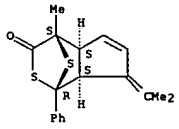


AB Cycloaddn. of fulvenes I (R = R1 = Me; R = H, R1 = OAc) with mesoionic compds. II (R2 = Ph, Me, H) in C6H6 at room temperature for 28-48 h gave the regio- and stereoselective [4π+2π] adducts III (R-R2 as before) in 3.1-49% yield. No periselectivity was observed with the unsym. fulvenes. Several other mesoionic ring systems failed to react or gave complex reaction products.

IT 99315-13-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

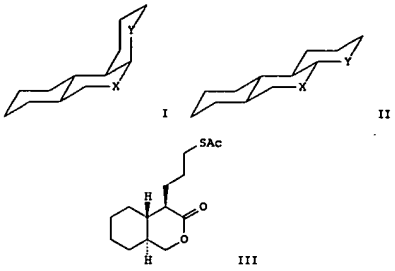
RN 99315-13-6 CAPLUS
CN 1,4-Epithiocyclopenta[c]thiopyran-3(1H)-one, 4,4a,7,7a-tetrahydro-4-methyl-7-(1-methylethylidene)-1-phenyl-, (1α,4α,4aβ,7aβ)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:5803 CAPLUS
DOCUMENT NUMBER: 104:5803
TITLE: Synthesis and equilibrium of conformationally rigid cis and trans tricyclic mono and dithioacetals. An evaluation of stereoelectronic (anomeric) effects in thioacetals
AUTHOR(S): Deslongchamps, Pierre; Guay, Daniel
CORPORATE SOURCE: Fac. Sci., Univ. Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.
SOURCE: Canadian Journal of Chemistry (1985), 63(10), 2757-62
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:5803
GI



I II

III

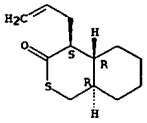
AB The synthesis of cis and trans tricyclic thioacetals I and II (X = O, Y = S; X = S, Y = O; X = Y = S) is reported. Thus, the bicyclic lactone III was reduced with dibal and the resulting thiol cyclized by p-MeC6H4SO3H to give I and II (X = O, Y = S). The cis isomers I are the kinetic products of cyclization, a result which is explained on the basis of stereoelectronic principles. Equilibration studies led to an evaluation of the anomeric effect for sulfur; it was found to be of the same order as that for oxygen.

IT **99410-28-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)

RN 99410-28-3 CAPLUS
CN 3H-2-Benzothiopyran-3-one, octahydro-4-(2-propenyl)-, (4α,4aα,8aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

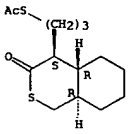
L4 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **99410-32-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reduction, and intramol. cyclization of, tricyclic dithioacetals from)

RN 99410-32-9 CAPLUS
CN Ethanethioic acid, S-[3-(octahydro-3-oxo-1H-2-benzothiopyran-4-yl)propyl] ester, (4α,4aα,8aβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1985:6124 CAPLUS
DOCUMENT NUMBER: 102:6124
TITLE: Intramolecular Diels-Alder reaction of iminothiol esters
AUTHOR(S): Tamaru, Yoshinao; Ishige, Osamu; Kawamura, Shinichi; Yoshida, Zenichi
CORPORATE SOURCE: Dep. Synth. Chem., Kyoto Univ., Kyoto, 606, Japan
SOURCE: Tetrahedron Letters (1984), 25(33), 3583-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:6124
GI

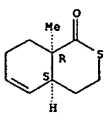
I

AB Diels-Alder reaction of dienyl α-methacrylthioimidates has been investigated under thermal or Lewis acid or protonic acid-catalyzed conditions. The utility of the reaction is shown by desulfurative ring contraction of the bicyclo[4.4.0] to the bicyclo[4.3.0] system. Thus, treatment of CH2:CHCH:CHCH2CH2SC(:NCMe3)CMe:CH with 1.5 N HCl at room temperature gave 85% I (X = S, X1 = NCMe3) which was converted to I (X = bond, X1 = O) in 6 steps.

IT **93472-08-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, transesterification, and alkylation of)

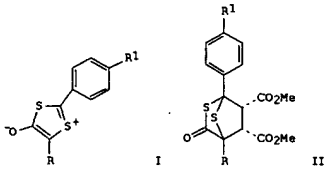
RN 93472-08-3 CAPLUS
CN 1H-2-Benzothiopyran-1-one, 3,4,4a,7,8,8a-hexahydro-8a-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

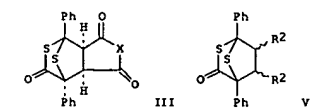


L4 ANSWER 22 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:615311 CAPLUS
DOCUMENT NUMBER: 89:215311
TITLE: [3 + 2]Cycloaddition reactions of mesoionic 1,3-dithiolones to ethylenedicarboxylic acid derivatives and 1,2-dibenzoylethylene
AUTHOR(S): Gotthardt, Hans; Christl, Brigitte
CORPORATE SOURCE: Gesamthochsch. Wuppertal, Wuppertal, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1978), 111(9), 3029-36
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I II



III V

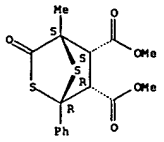
AB Dithiolium compds. I (R = Ph, Me; R1 = H, Me, MeO) added to (Z)-MeO2CCH:CHCO2Me to give II. Cycloaddn. of I [R = Ph, R1 = H (III)] with maleic anhydride gave IV, (X = O), whereas the cycloaddn. with N-phenylmaleimide gave a mixt of IV (X = NPh) and the corresponding endo-isomer. Treating III with (E)-R2CH:CHR2 (R2 = PhCO, CO2Me) gave mixed trans isomers of V.

IT **68145-44-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 68145-44-8 CAPLUS
CN 2,7-Dithiabicyclo[2.2.1]heptane-5,6-dicarboxylic acid, 4-methyl-3-oxo-1-phenyl-, dimethyl ester, (endo,endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 22 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



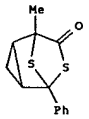
L4 ANSWER 23 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:597420 CAPLUS
DOCUMENT NUMBER: 89:197420
TITLE: Cycloaddition reactions of mesoionic 1,3-dithiolones to cyclic olefin derivatives
AUTHOR(S): Gotthardt, Hans; Weisshuhn, C. Michael; Christl, Brigitte
CORPORATE SOURCE: Gesamthochsch. Wuppertal, Wuppertal, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1978), 111(9), 3037-47
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 89:197420
GI For diagram(s), see printed CA Issue.

AB Treating dithiolium compound I (R = Ph; R1 = H) with cyclopropene, acenaphthylene, and benzoquinone gave II, III, and IV, resp.; IV also fragment to give benzo[c]thiophene-4,7-diones. Similar adducts were prepared from I (R = Ph, R1 = Me, H) and norbornene, norbornadiene, cyclopentene, cyclopentadiene, 1,3-cyclohexadiene, or 1,5-cyclooctadiene.

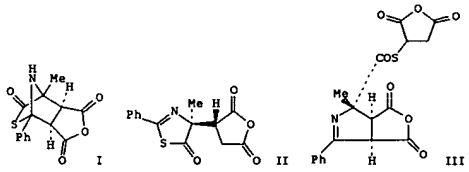
IT 68145-11-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 68145-11-9 CAPLUS
CN 6,8-Dithiatricyclo[3.2.1.02,4]octan-7-one, 1-methyl-5-phenyl-, (1α,2β,4β,5α)- (9CI) (CA INDEX NAME)



L4 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:432910 CAPLUS
DOCUMENT NUMBER: 85:32910
TITLE: Addition reactions of thiazol-5(4H)-ones. II. Cycloaddition and Michael addition reactions of 4-substituted 2-phenylthiazol-5(4H)-ones
AUTHOR(S): Barrett, G. C.; Walker, R.
CORPORATE SOURCE: Oxford Polytech., Oxford, UK
SOURCE: Tetrahedron (1976), 32(5), 571-7
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:32910
GI

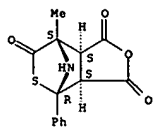


AB The mixts. of adducts formed under mild conditions between 4-substituted 2-phenylthiazol-5(4H)-ones and electron-deficient alkenes include stable cycloadducts, Michael adducts formed through C-2 or C-4 of the thiazolone, and 1:2 adducts. E.g., 4-methyl-2-phenylthiazol-5(4H)-one with maleic anhydride gave 32% I, 15% II, and 10% III; in the presence of a trace of NaOH II (45%) was the only product. III is formed by reaction of I with maleic anhydride. Products formed by extrusion of COS from cycloadducts are the same as those formed from the analogous oxazolone. Addition reactions of thiazolones and oxazolones with dipolarophiles are compared.

IT 60027-22-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with maleic anhydride)

RN 60027-22-7 CAPLUS
CN 3H-Thiopyrano[3,4-c]furan-4,7-imine-1,3,6-trione, tetrahydro-7-methyl-4-phenyl-, (3aα,4β,7β,7aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

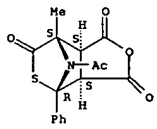


L4 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT 60027-06-7P 60027-08-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

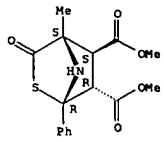
RN 60027-06-7 CAPLUS
CN 3H-Thiopyrano[3,4-c]furan-4,7-imine-1,3,6-trione, 8-acetyltetrahydro-7-methyl-4-phenyl-, (3aα,4β,7β,7aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 60027-08-9 CAPLUS
CN 2-Thia-7-azabicyclo[2.2.1]heptane-5,6-dicarboxylic acid, 4-methyl-3-oxo-1-phenyl-, dimethyl ester, (1α,4α,5α,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:466129 CAPLUS
DOCUMENT NUMBER: 79:66129
TITLE: Synthesis of thiabicyclo[2.2.2]octenes. Carbon-13 nuclear magnetic resonance spectra of bicyclic sulfides
AUTHOR(S): Reich, Hans J.; Trend, John E.
CORPORATE SOURCE: Dep. Chem., Univ. Wisconsin, Madison, WI, USA
SOURCE: Journal of Organic Chemistry (1973), 38(15), 2637-40
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2-Thiabicyclo[2.2.2]oct-5-ene (I) was prepared by 1,4-addition of thiophosgene to 1,3-cyclohexadiene giving 3,3-dichloro-2-thiabicyclo-[2.2.2]oct-5-ene (II) followed by reduction with LiAlH4. 7,7-Dimethyl-2-thiabicyclo[2.2.2]oct-5-ene and 4,6,7,7-tetramethyl-2-thiabicyclo[2.2.2]oct-5-ene (III) were similarly prepared from 5,5-dimethyl- and 1,3,5,5-tetramethyl-1,3-cyclohexadiene. I was characterized by diimide reduction to the known 2-thiabicyclo[2.2.2]octane which was not the photolysis product of 3-cyclohexenylmethanethiol as previously reported (J. M. Surzur et al., 1971). III was characterized by oxidation to the S-oxide and S,S-dioxide. Hydrolysis of II gave 2-thiabicyclo[2.2.2]oct-5-en-2-one. The structures were established by 13C NMR.

IT **40169-02-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40169-02-6 CAPLUS
CN 2-Thiabicyclo[2.2.2]oct-5-en-3-one, 4,6,7,7-tetramethyl- (9CI) (CA INDEX NAME)